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ARMY MOBILITY EQUIPMENT RESEARCH AND DEVELOPMENT COMM--ETC F/G 14/2
FUNDAMENTALS OF ION MOTION IN ELECTRIC RADIOFREQUENCY MULTIPOLE--ETC(U)
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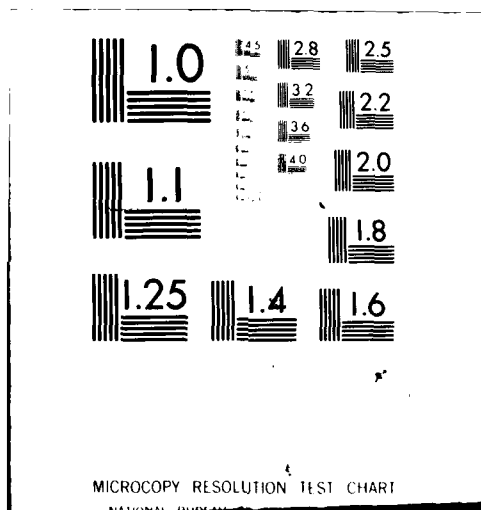
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Report 2332

FUNDAMENTALS OF ION MOTION IN ELECTRIC
RADIOFREQUENCY MULTIPOLE FIELDS

by

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July 1981

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 2332	2. GOVT ACCESSION NO. AD-A107	3. RECIPIENT'S CATALOG NUMBER 24
4. TITLE (and Subtitle) FUNDAMENTALS OF ION MOTION IN ELECTRIC RADIOFREQUENCY MULTIPOLE FIELDS		5. TYPE OF REPORT & PERIOD COVERED Final: April 1981
7. AUTHOR(s) M.H. Friedman (MERADCOM); A.L. Yergey (NIH); J.E. Campana (NRL); L. Kelner (NIH)		6. PERFORMING ORG. REPORT NUMBER
9. PERFORMING ORGANIZATION NAME AND ADDRESS US Army Mobility Equipment Research and Development Command; ATTN: DRDME-ND; Fort Belvoir, VA 22060		8. CONTRACT OR GRANT NUMBER(s)
11. CONTROLLING OFFICE NAME AND ADDRESS US Army Mobility Equipment Research and Development Command; ATTN: DRDME-ND; Fort Belvoir, VA 22060		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 11
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) 19		12. REPORT DATE July 1981
		13. NUMBER OF PAGES 43
		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number)		
Mass Filter	Hexapole	Electromagnetic Fields
Mass Spectrometry	Octapole	Maxwell Equations
Mass Spectrometer	Decapole	Lorentz Force
Mass Spectroscopy	Ion Motion	
Quadrupole	Radiofrequency	
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)		
<p>➤ The fundamentals of ion motion in electromagnetic fields are reviewed in detail with a special emphasis on electric radiofrequency (RF) fields which are used frequently in dynamic mass spectrometry. Forces and effects on ions in electromagnetic fields which are typically neglected, but which may be important in practical</p> <p>(Continued)</p>		

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applications, are reviewed and discussed for completeness. A method based on complex variable theory is developed for finding the potential function of "ideal multipole electromagnetic fields." Application of this method for the determination of potential functions and differential equations of ion motion is demonstrated with reference to the electric radiofrequency dipole, quadrupole, hexapole, octapole, and decapole fields. The results and implications of this preliminary communication and tutorial are of importance in ion physics and dynamic mass spectrometry.

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FUNDAMENTALS OF ION MOTION IN ELECTRIC RADIOFREQUENCY MULTIPOLE FIELDS

I. INTRODUCTION

The strong-focusing effect, which utilizes alternating electromagnetic fields, is the basis for high-energy accelerator physics¹ and quadrupole mass spectrometry.² Ion motion through such electromagnetic fields, induced by arbitrary-shaped pole pieces,³ cannot be described in closed mathematical form. However, the differential equations describing ion motion through the electromagnetic field induced by voltages on an electrode structure employing hyperbolic-shaped electrodes can be written in an analytic form which is known as the Mathieu equation, the theory and properties of which are well known.⁴⁻⁷ Therefore, it is not surprising that many mass filters are based on electrodes with a hyperbolic geometry.

The methods for obtaining the potential functions and the differential equations of ion motion in time-varying electromagnetic fields are probably familiar to accelerator physicists and electrical engineers. Surprisingly, a search of the literature has failed to reveal a fundamental and practical discussion of this subject suitable to those researchers, such as mass spectrometrists and ion physicists, who might benefit most by such a discussion.

Research on mass filters has been confined primarily to the quadrupole, the monopole, the three-dimensional quadrupole, and approximations to these three.⁷⁻⁹ It may be possible that electric radiofrequency mass filters with desirable properties could be implemented if electrode geometries other than the above were considered.

¹ E. D. Courant, M. S. Livingston, and H. S. Snyder, *Phys. Rev.*, **88**, 1190 (1952); J. D. Blewett, *Phys. Rev.*, **88**, 1197 (1952).

² W. Paul and H. Steinwedel, *Z. Naturforsch. Teil A.*, **8**, 448 (1953); W. Paul, H. P. Reinhard, and U. von Zahn, *Z. Phys.*, **152**, 143 (1958).

³ The terms conductor, electrodes, and pole pieces will be used interchangeably.

⁴ F. M. Arscott, *Periodic Differential Equations*, The Macmillan Co., New York (1964).

⁵ N. W. McLachlan, *Theory and Application of Mathieu Functions*, Oxford University Press, New York (1947).

⁶ Computation Laboratory, *Tables Relating to Mathieu Functions*, U.S. Bureau of Standards, Columbia University Press, New York (1951).

⁷ P. H. Dawson (Editor), *Quadrupole Mass Spectrometry and Its Applications*, Elsevier, Amsterdam (1976).

⁸ J. F. J. Todd and G. Lawson, *MTP International Review of Science, Physical Chemistry, Mass Spectrometry, Series Two*, Vol. 5, edited by A. Maccoll, Butterworths, London (1975).

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, **33**, 101 (1980) and references cited within.

Previous work with the quadrupole mass filter electrode geometry has been directed towards making circular cross section electrode approximations to "ideal" hyperbolic cross section electrodes. Denison¹⁰ has pointed out a propagation of errors in the literature that deal with the correct positioning of cylindrical electrodes to approximate a hyperbolic electrostatic field. Denison presented the equations of ion motion in such fields and he reported variations in the stability diagrams resulting from the relative positioning of the cylindrical electrodes approximating ideal hyperbolic cross section electrodes. Denison discusses the power series expansion expression for the quadrupole potential distribution which is obtained by considering a point charge located in a quadrupole field formed by electrodes of line charge.¹¹ Successive terms in the series expression represent quadrupole, dodecapole, icosapole geometries, etc. A commercial instrument,¹² employing correcting electrodes to account for the dodecapole field distortions was available for a number of years but ultimately was replaced in favor of electrodes with hyperbolic cross sections.

Although the quadrupole geometry has been used for the mass filter in practice, there is the possibility that other geometries might give equivalent or superior resolution for a given transmission and might provide other advantages as well. New geometries could be investigated empirically, but for practical reasons this task requires a means of evaluating electrode geometry designs theoretically. In this report, several alternatives to the quadrupole geometry are considered and equations of ion motion in closed analytical form are derived for each of them. By detailed consideration of these particular geometries it may be possible that insight into the characteristics of a useful mass filter geometry will be gained.

The first objective of this report is to present the fundamental laws of physics and the approximations which govern ion motion through electromagnetic fields in the electric RF mass filter. A second objective is to present a method for finding the potential function of an arbitrary "ideal multipole field" and, subsequently, the differential equations of motion for an ion traversing such a field. A summary and discussion of forces and effects which are typically neglected in the physics of ion motion, but which may be important under certain circumstances, are included for completeness. Finally, the potential functions and differential equations which describe ion motion in the electric RF dipole, quadrupole, hexapole, octapole, and decapole fields are derived using mathematical methods. This is a first step toward investigating the properties of alternative multipole geometries for mass filters.

¹⁰ D. R. Denison, *J. Vac. Sci. Technol.*, 8, 266 (1971).

¹¹ See H. Matsuda and T. Matsuo, *Int. J. Mass Spectrom. Ion Physics*, 24, 107 (1977), for a partial derivation of the power series expansion.

¹² Hewlett-Packard Corporation, Palo Alto, CA.

II. FUNDAMENTAL PHYSICS OF IONS IN ELECTROMAGNETIC FIELDS

The electric RF strong-focusing effect has been employed in quadrupole mass spectrometry for over twenty years.^{2,9} The theory of operation for this versatile device has been discussed by many authors⁷⁻⁹ and in all discussions it appears that the fundamental physics underlying ion motion in electromagnetic fields has been assumed.

In this section, a method for finding the differential equation governing the motion of an ion through electromagnetic fields with any number of arbitrary-shaped pole pieces is derived. This derivation, while general, is directed specifically to ion motion through an electric RF field which finds popular use as a mass filtering device.

The differential equation which describes the motion of an ion through a field is obtained from Newton's law of motion

$$\mathbf{F} = m \frac{d^2 \mathbf{r}}{dt^2}, \quad (1)$$

where \mathbf{F} is the force on the ion, m is the mass of the ion and \mathbf{r} is the radius vector from the origin. The force on an ion with charge e moving through an electric field \mathbf{E} and a magnetic field \mathbf{B} with a velocity \mathbf{v} is given by the Lorentz force law

$$\mathbf{F} = e (\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (2)$$

It is necessary to compute the \mathbf{E} and \mathbf{B} fields from the time-varying potential imposed on the pole pieces to find the motion of the ions from Equations 1 and 2. These are computed from the general Maxwell equations:

$$\begin{aligned} \nabla \cdot \mathbf{D} &= \rho & \nabla \times \mathbf{E} &= - \frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{B} &= 0 & \nabla \times \mathbf{H} &= \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, \end{aligned} \quad (M1)$$

where ρ is the real charge density in the medium and \mathbf{J} is the current per unit area in the medium.

² W. Paul and H. Steinwedel, *Z. Naturforsch. Teil A.*, **8**, 448 (1953); W. Paul, H. P. Reinhard, and U. von Zahn, *Z. Phys.* **152**, 143 (1958).

⁷ P. H. Dawson (Editor), *Quadrupole Mass Spectrometry and Its Applications*, Elsevier, Amsterdam (1976).

⁸ J. F. J. Todd and G. Lawson, *MTP International Review of Science, Physical Chemistry, Mass Spectrometry*, Series Two, Vol. 5, edited by A. Maccoll, Butterworths, London (1975).

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, **33**, 101 (1980) and references cited within.

The del operator ∇ which appears in Equations M1 can be defined by

$$\nabla\phi \cdot d\mathbf{r} = d\phi, \quad (3)$$

where ϕ is a scalar function of position, $d\phi$ is the total differential of ϕ , and $d\mathbf{r}$ is the total differential of the radius vector \mathbf{r} . This definition can be used to find an explicit representation of the operator ∇ in rectangular coordinates. From elementary calculus:

$$d\phi = \frac{\partial\phi}{\partial x} dx + \frac{\partial\phi}{\partial y} dy + \frac{\partial\phi}{\partial z} dz.$$

In rectangular coordinates the displacement $d\mathbf{r}$ is

$$d\mathbf{r} = \hat{i}dx + \hat{j}dy + \hat{k}dz.$$

Since dx , dy , and dz are independent, in rectangular coordinates $\nabla\phi$ is identified as

$$\nabla\phi = \hat{i}\frac{\partial\phi}{\partial x} + \hat{j}\frac{\partial\phi}{\partial y} + \hat{k}\frac{\partial\phi}{\partial z}$$

and the operator ∇ is identified as

$$\nabla = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}, \quad (4)$$

where \hat{i} , \hat{j} , and \hat{k} are unit vectors along the x , y , and z axis. Expressions for the ∇ operator in co-ordinate systems other than the rectangular one are given elsewhere.^{13 14}

Equations 1 and 2 and Maxwell's equations M1 are fundamental equations which describe the motion of an ion through any electromagnetic field. What do these equations mean? Suppose that the charge density $\rho(x,y,z,t)$ and the current density $\mathbf{J}(x,y,z,t)$ are known throughout space and for all time. With ∇ defined in Equation 4, the divergence, curl, and the time derivative of all the quantities in Equations M1 can be readily computed providing $\mathbf{E}(x,y,z,t)$, $\mathbf{D}(x,y,z,t)$, $\mathbf{B}(x,y,z,t)$, and $\mathbf{H}(x,y,z,t)$ are specified. Maxwell's equations assert that the \mathbf{E} , \mathbf{D} , \mathbf{B} , and \mathbf{H} fields cannot be chosen arbitrarily and must be chosen in such a way that they satisfy Equations M1. Furthermore, the \mathbf{E} and \mathbf{D} fields are related and the \mathbf{B} and \mathbf{H} fields are related by the properties of matter.

¹³ E. M. Pugh and E. W. Pugh, *Principles of Electricity and Magnetism*, Addison-Wesley Publishing Co., Reading, MA (1960).

¹⁴ S. Ramo, J. R. Whinnery, and T. Van Duzer, *Fields and Waves in Communication Electronics*, John Wiley and Sons, Inc., New York (1965).

The vector \mathbf{D} (called the electric displacement vector) is related to the vector \mathbf{E} by^{13 14}

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \quad (5)$$

where ϵ_0 is a constant called the permittivity of free space and \mathbf{P} is a polarization vector characteristic of a particular material. In linear, homogeneous, isotropic materials,^{13 14} $\mathbf{P} = \epsilon_0 \chi_e \mathbf{E}$ (χ_e is a dimensionless quantity called the polarizability or electric susceptibility) so that Equation 5 becomes

$$\mathbf{D} = (\epsilon_0 + \epsilon_0 \chi_e) \mathbf{E} = \epsilon \mathbf{E}. \quad (6)$$

The constant ϵ in the last equation, the permittivity, depends only on the medium in which the field exists. Similarly, \mathbf{H} (called the magnetic field intensity or magnetic field strength vector) is related to \mathbf{B} by¹³

$$\mathbf{B} = \mu_0 \mathbf{H} + \mathbf{m}, \quad (7)$$

where μ_0 is a constant (called the permeability of free space) and \mathbf{m} is called a magnetic polarization vector.¹⁵ In linear, homogeneous, isotropic materials $\mathbf{m} = \mu_0 \chi_m \mathbf{H}$ (the dimensionless quantity χ_m is called the magnetic susceptibility of the material under consideration) so that Equation 7 becomes

$$\mathbf{B} = \mu \mathbf{H}. \quad (8)$$

The constant μ in Equation 8, called the permeability, depends only on the medium in which the field exists. Thus for linear, homogeneous, isotropic media, Maxwell's Equations M1 must be satisfied subject to the constraints of Equations 6 and 8.

With these assumptions (Equations 6 and 8) about the properties of the material from which pole pieces are constructed and for the medium in which the ion moves, Maxwell's equations M1 become:¹⁶

¹³ E. M. Pugh and E. W. Pugh, *Principles of Electricity and Magnetism*, Addison-Wesley Publishing Co., Reading, MA (1960).

¹⁴ S. Ramo, J. R. Whinnery, and T. Van Duzer, *Fields and Waves in Communication Electronics*, John Wiley and Sons, Inc., New York (1965).

¹⁵ Some authors write Equation 7 in the form $\mathbf{B} = \mu(\mathbf{H} + \mathbf{M})$ and call \mathbf{M} the magnetization. This allows the units of \mathbf{H} and \mathbf{M} to be the same. The form of Equation 7 is used here to emphasize the similarity with Equation 5.

¹⁶ Here Maxwell's equations are expressed in terms of \mathbf{E} and \mathbf{B} rather than \mathbf{D} and \mathbf{H} since \mathbf{E} and \mathbf{B} are the vectors in Equation 2.

$$\begin{aligned}
\nabla \cdot (\epsilon \mathbf{E}) &= \rho & \nabla \times \mathbf{E} &= - \frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 & \nabla \times \frac{\mathbf{B}}{\mu} &= \mathbf{J} + \frac{\partial(\epsilon \mathbf{E})}{\partial t}
\end{aligned}
\tag{M2}$$

Since the ion of interest is moving in free space (vacuum), ϵ and μ have the constant values ϵ_0 and μ_0 in Equations 6 and 8. If the charges of ions and the associated current densities can be neglected for the purpose of computing the \mathbf{E} and \mathbf{B} fields acting on them, Maxwell's Equations M2 become:

$$\begin{aligned}
\nabla \cdot \mathbf{E} &= 0 & \nabla \times \mathbf{E} &= - \frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 & \nabla \times \frac{\mathbf{B}}{\mu_0} &= \frac{\partial(\epsilon_0 \mathbf{E})}{\partial t}
\end{aligned}
\tag{M3}$$

Now suppose that the \mathbf{E} and \mathbf{B} fields are not changing with time. For this situation, Maxwell's Equations M3 become:

$$\begin{aligned}
\nabla \cdot \mathbf{E} &= 0 & \nabla \times \mathbf{E} &= 0 \\
\nabla \cdot \mathbf{B} &= 0 & \nabla \times \mathbf{B} &= 0.
\end{aligned}
\tag{M4}$$

The validity of the different forms of Maxwell's Equations (M1, M2, M3, M4) merits discussion. Maxwell's Equations in the form of Equations M1 are universally valid in any medium. Maxwell's Equations M2 are valid without approximation for electromagnetic fields within a vacuum where the \mathbf{E} and \mathbf{D} fields are parallel and the \mathbf{B} and \mathbf{H} fields are parallel. This condition is fulfilled when the fields exist in linear, homogeneous, isotropic materials and for such material Equations M2 are a valid approximation. Thus in all regions of a mass filter that are linear, isotropic, and homogeneous (i.e., within the pole pieces and in the vacuum enclosed by them) Maxwell's Equations M2 are valid. In a mass filter, the vacuum conditions approximate free space so that the permittivity ϵ and permeability μ should be well approximated by ϵ_0 and μ_0 . Furthermore, with a low enough density of ions, ρ and \mathbf{J} will approach zero, and therefore Maxwell's Equations M3 are a good approximation in the vacuum region enclosed by the pole pieces of a mass filter. However, in a mass filter, the voltages on the electrodes change at radiofrequencies resulting in \mathbf{B} and \mathbf{E} fields which will also change at the same frequencies, so it is not obvious that Maxwell's Equations M4 are valid in the vacuum region enclosed by the pole pieces. The use of Equations M4 in this region can be understood through the following discussion. Equations M3 predict¹³ that $B_0 = E_0/c$

¹³ E. M. Pugh and E. W. Pugh, *Principles of Electricity and Magnetism*. Addison-Wesley Publishing Co., Reading, MA (1960).

where B_0 and E_0 are the maximum amplitudes of the \mathbf{B} and \mathbf{E} fields and c is the speed of light where $c = (\epsilon_0 \mu_0)^{-1/2}$. Thus the \mathbf{B} field in the Lorentz force law (Eq. 2) exerts a negligible force on the ion compared to the \mathbf{E} field unless the ion is moving at a speed comparable to the speed of light. The fastest ions in a quadrupole mass filter are moving slowly ($v/c < 10^{-4}$) compared to the speed of light, even under extreme operating conditions. Therefore, it is not necessary to consider the \mathbf{B} fields any further for the purpose of computing the force on an ion. The Lorentz force law (Equation 2) reduces to

$$\mathbf{F} = e\mathbf{E}, \quad (9)$$

while Maxwell's Equations M4 become:

$$\nabla \cdot \mathbf{E} = 0 \quad \nabla \times \mathbf{E} = 0. \quad (M5)$$

The second of these Equations M5 is valid only for an alternating potential which has a frequency ν low enough such that

$$\lambda = c/\nu \gg \ell. \quad (10)$$

That is, the wavelength λ associated with the electromagnetic wave must be much greater than the length ℓ of the electrode structure. The necessity of Equation 10 can be understood in the following way. If the wavelength does not satisfy Equation 10 there is a possibility of standing waves (just as in the case of sound waves in an organ pipe) and these are not predicted by Equations M5. Typically, the length of the mass filter is less than 1 m and the frequencies used are well below 10 MHz.⁹ Therefore, Equations 9 and M5 are valid for the vacuum region traversed by the ions in the mass filter.

An \mathbf{E} field which satisfies Maxwell's Equations M5 can be found with the aid of two mathematical theorems. Stokes theorem, valid for any continuous, differentiable vector field \mathbf{A} , asserts that

$$\int_S \nabla \times \mathbf{A} \cdot d\mathbf{s} = \oint \mathbf{A} \cdot d\mathbf{r}, \quad (11)$$

where $d\mathbf{r}$ is a vector on the circumference of the enclosed area S and whose direction is in the direction of the integration. The vector $d\mathbf{s}$ has a magnitude equal to the area ds , and its direction is normal to ds . The ambiguity in the two directions normal to ds is resolved by the right-hand rule, that is $d\mathbf{s}$ points in the direction of the thumb with the other fingers of the right hand pointing in the direction $d\mathbf{r}$. In Equation 11, the integral on the

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, 33, 101 (1980) and references cited within.

right is over the entire circumference and the integral on the left is over the area S enclosed by the circumference. Stokes theorem enables a two-dimensional integral over a surface which has the form given on the left side of Equation 11 to be evaluated by the simpler one-dimensional integral on the right-hand side of Equation 11. Application of Stokes theorem to the second of Equations M5 implies

$$\oint \mathbf{E} \cdot d\mathbf{r} = 0 \quad (12)$$

over any closed path which defines a surface over which $\nabla \times \mathbf{E} = 0$.

The second mathematical theorem asserts that any vector field \mathbf{E} , which has the property that $\oint \mathbf{E} \cdot d\mathbf{r} = 0$ around every closed path, can be represented as the divergence of a scalar field $\phi(x,y,z)$, that is

$$\mathbf{E} = -\nabla \phi(x,y,z). \quad (13)$$

The minus sign in Equation 13 is not essential and is included to conform with convention. This is analogous to the situation in classical mechanics where the potential energy $U(\mathbf{r})$ is defined so that $\mathbf{F} = -\nabla U(\mathbf{r})$. The scalar field $\phi(x,y,z)$ is called the potential function. Equation 13 states that a vector field, which normally needs three scalar fields to represent it (one for each component), can be represented by a single scalar field if Equation 12 is satisfied for every closed path.

The validity of Equation 13 in a region of space for which Equation 12 is satisfied for every closed path is seen by the following argument. Equation 12 applied to Figure 1 implies

$$\int_{ABC} \mathbf{E} \cdot d\mathbf{r} + \int_{CDA} \mathbf{E} \cdot d\mathbf{r} = 0, \quad (14)$$

where the letters on the bottom of the integral symbol indicate the path of the integration. If the direction of a line integral is reversed, then the sign changes such that

$$\int_{CDA} \mathbf{E} \cdot d\mathbf{r} = -\int_{ADC} \mathbf{E} \cdot d\mathbf{r}$$

and Equation 14 becomes

$$\int_{ABC} \mathbf{E} \cdot d\mathbf{r} = \int_{ADC} \mathbf{E} \cdot d\mathbf{r}. \quad (15)$$

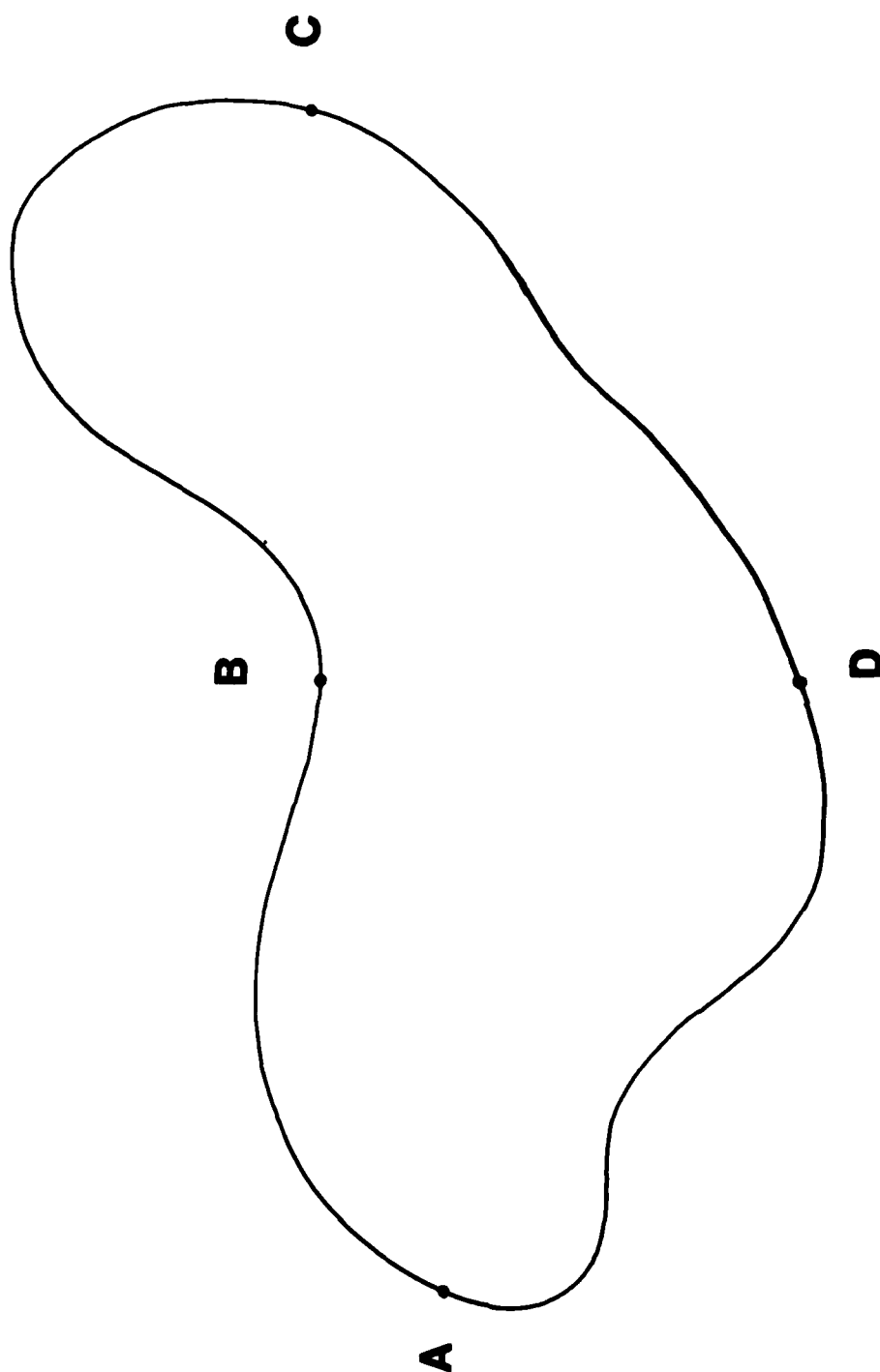


Figure 1. Vector fields and gradients.
If the line integral of a vector field $E(x,y,z)$ around any closed path is zero, then there exists a scalar quantity $\phi(x,y,z)$ a function of position only with the property $E = -\nabla\phi$.

Equation 15 states that if Equation 12 is valid then the line integral from A to C is independent of the path. Thus if Equation 12 is valid, then the integral from point A to point C can only depend on the coordinates of points A and C.

$$\int_{ABC} \mathbf{E} \cdot d\mathbf{r} = -[\phi(\mathbf{r}_C) - \phi(\mathbf{r}_A)]. \quad (16)$$

The function ϕ called the potential, corresponds to the voltage on the poles of the electrode structure. Now suppose points A and C are taken close together, then Equation 16 becomes

$$\mathbf{E} \cdot d\mathbf{r} = -d\phi = -\nabla\phi \cdot d\mathbf{r}, \quad (17)$$

where the last equality follows from the definition of $\nabla\phi$ (Eq. 3). Since Equation 17 is true for any element of length $d\mathbf{r}$, there exists a function ϕ which depends only on the position such that Equation 13 is true. This completes the proof of Equation 13.

Substituting \mathbf{E} from Equation 13 into the first equation of Equations M5 gives

$$\nabla \cdot \nabla\phi(x,y,z) = 0. \quad (18)$$

The symbol $\nabla \cdot \nabla$ is called the Laplacian and is denoted by ∇^2 ; consequently, Equation 18 becomes

$$\nabla^2\phi(x,y,z) = 0. \quad (19)$$

Equation 19 is called Laplace's equation and in rectangular coordinates

$$\begin{aligned} \nabla^2 &= \nabla \cdot \nabla \\ &= \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \cdot \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \\ &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \end{aligned}$$

Expressions for ∇^2 in the cylindrical and spherical coordinate systems are given elsewhere.^{13 14} Since Equation 19 is a consequence of Maxwell's Equations M5, it is apparent that if a function $\phi(x,y,z)$ can be found which satisfies Equation 19, then the E field defined by Equation 13 will satisfy Maxwell's Equations M5.

The prescription for finding the differential equation of ion motion for any configuration of pole pieces can now be given. Suppose that an ion is moving in the field of a set of n conductors each at a constant voltage $\phi_i (i = 1, 2, \dots, n)$. Let $z = f_i(x,y)$ denote the equation for the surface of the i th conductor. The differential equation of motion can be found by obtaining a potential function $\phi(x,y,z)$ which satisfies Laplace's equation (Equation 19) and which also satisfies the boundary conditions

$$\phi(x,y,f_i(x,y)) = \phi_i \quad (i = 1, 2, \dots, n). \quad (20)$$

This latter requirement says that the potential function must be equal to the voltage applied to any of the electrodes at the electrode surfaces.

Generally, it is difficult to find such a function which satisfies Equations 19 and 20. The function $\phi(x,y,z)$ can sometimes be found analytically using the method of images,^{13 14 17} complex variable theory,^{13 14 17 18} infinite series expansions^{13 14 17 19} or it can be evaluated numerically using digital computers.^{20 21}

¹³ E. M. Pugh and E. W. Pugh, *Principles of Electricity and Magnetism*, Addison-Wesley Publishing Co., Reading, MA (1960).

¹⁴ S. Ramo, J. R. Whinnery, and T. Van Duzer, *Fields and Waves in Communication Electronics*, John Wiley and Sons, Inc., New York (1965).

¹⁷ J. D. Jackson, *Classical Electrodynamics*, John Wiley and Sons, Inc., New York (1962).

¹⁸ R. V. Churchill, *Complex Variables and Applications*, McGraw-Hill Book Co., Inc., New York (1960).

¹⁹ R. V. Churchill, *Fourier Series and Boundary Value Problems*, McGraw-Hill Book Co., Inc., New York (1941).

²⁰ K. J. Binns and P. J. Lawrenson, *Analysis and Computation of Electric and Magnetic Field Problems*, The Macmillan Co., New York (1963).

²¹ M. L. Baron and M. G. Salvadori, *Numerical Methods in Engineering*, Prentice-Hall, Inc., Englewood Cliffs, NJ (1964).

Once the potential $\phi(x,y,z)$ is known, the differential equation of motion can be found using Newton's law of motion

$$F = m \frac{d^2 r}{dt^2} = -e \nabla \phi(x, y, z). \quad (21)$$

As discussed earlier, this method is approximately valid for time-varying potentials²²

$$\phi_i = \phi_{DC} - \phi_{AC} \cos \omega t. \quad (22)$$

providing the potential does not change too rapidly with time (i.e., subject to the limitations of Equations M5 and 10). Physically, Equation 22 corresponds to subjecting the electrodes to a voltage which has both d.c. and a.c. components.

The remainder of this report will consider only infinitely long conductors whose shape does not vary with z . Although real electrode structures must necessarily be of finite length, this approximation is made because it captures the essential features for the operation of electric RF devices while avoiding some of the mathematical complexities. With this approximation, the potential for such a conductor configuration does not depend on z ; i.e., $\phi(x,y,z) = \phi(x,y)$ and hence the force in the z -direction is zero; i.e.,

$m \frac{d^2 z}{dt^2} = 0$. The equation of motion in the z -direction can be integrated directly

$$z = v_{z_0} t + z_0 \quad (23)$$

Here v_{z_0} and z_0 are the z -component of velocity and the z -coordinate respectively at $t=0$.

III. METHOD FOR OBTAINING POTENTIAL FUNCTIONS AND EQUATIONS OF ION MOTION IN MULTIPOLE FIELDS

The approach of the previous section was to find the potential function $\phi(x,y,z)$ for a specified set of conductors at potentials ϕ_i . An alternative approach to the problem is to find a function $U_n(x,y)$ which satisfies Laplace's equation (Equation 19) and from this function determine the equipotential surfaces of the pole pieces. If conductors with given applied potentials are fashioned which coincide with the equipotential surfaces, a potential function

²² The minus sign in Equation 22 is not essential and is chosen by convention.

$$\phi(x,y) = K_n U_n(x,y) \quad (24)$$

can be found which satisfies Laplace's equation and the boundary conditions (Equation 20) by simply choosing the constant K_n properly. Physically, K_n is related to the dimension of the electrode structure and the applied electrode potentials; it is chosen such that $\phi(x,y)$ matches the known potentials at the equipotential surfaces.

Functions which satisfy Laplace's equation may be found by application of the theory of complex variables. If the complex variable $z = x + iy$ is raised to an integral power n , then the result can be expressed as the sum of two functions, a real $U_n(x,y)$ and an imaginary $V_n(x,y)$ part

$$(x + iy)^n = U_n(x,y) + iV_n(x,y). \quad (25)$$

The integer n defines the order of the multipole field. From complex variable theory z^n is known to be analytic and so the Cauchy-Riemann equations are applicable:¹⁸

$$\frac{\partial U_n(x,y)}{\partial x} = \frac{\partial V_n(x,y)}{\partial y} \quad (26a)$$

$$\frac{\partial U_n(x,y)}{\partial y} = -\frac{\partial V_n(x,y)}{\partial x} \quad (26b)$$

The sum of the partial derivative of the first of these equations with respect to x and the partial derivative of the second of these equations with respect to y gives

$$\frac{\partial^2 U_n(x,y)}{\partial x^2} + \frac{\partial^2 U_n(x,y)}{\partial y^2} = 0. \quad (27)$$

Thus the function $U_n(x,y)$ satisfies Laplace's equation.

The method described here for obtaining the potential function and the differential equation of motion can be summarized as follows.

¹⁸ R. V. Churchill, *Complex Variables and Applications*, McGraw-Hill Book Co., Inc., New York (1960).

A. Evaluate the function $U_n(x,y)$ for the variable z^n where n is any positive non-zero integer. The function $U_n(x,y)$ will satisfy Laplace's equation (Equation 27).

B. The equipotential conductor surfaces are constructed so that they fall on the locus of points in the (x,y) plane defined by $U_n(x,y) = \pm \text{constant}$. The separation between opposite electrodes is chosen to be $2r_0$ to insure that, for the case of the quadrupole, the standard quadrupole geometry² is reproduced. Geometrically adjacent conductors are arbitrarily chosen to have applied potentials of $\phi_i = \phi_0/2$ and $\phi_i = -\phi_0/2$, where ϕ_0 is allowed to vary with time (Equation 22), subject to those constraints put forth previously (the constraints of Equation 10 and the constraints associated with Equations M5). With the ϕ_i so defined, ϕ_0 is simply the voltage between any two adjacent electrodes.

C. An appropriate constant K_n is determined such that $K_n U_n(x,y) = \phi(x,y)$ satisfies the boundary conditions; i.e., K_n is chosen so that $\phi(x,y)$ matches the known potentials at the equipotential surfaces.

D. The differential equation of an ion is determined from the potential found in C using Newton's law of motion (Equation 21).

In brief, find a potential function $\phi(x,y)$ which satisfies Laplace's equation (Equation 19) and the boundary conditions (Equation 20); then ion motion is found from Newton's law of motion (Equation 21).

This method will be applied in Section V to obtain potential functions and differential equations of motion for various multipole electrode geometries.

IV. APPROXIMATIONS IN THE EQUATIONS FOR ION MOTION

Several approximations implicit in the prescription for finding the differential equations of ion motion given in the preceding section are a result of neglecting the various forces that ions may experience. These "idealized" equations of motion are normally used in describing ion motion.^{2 7-10} These approximations will now be explicitly discussed.

² W. Paul and H. Steinwedel, *Z. Naturforsch. Teil A.*, 8, 448 (1953); W. Paul, H. P. Reinhard and U. von Zahn, *Z. Phys.* 152, 43 (1958).

⁷ P. H. Dawson (Editor), *Quadrupole Mass Spectrometry and Its Applications*, Elsevier, Amsterdam (1976).

⁸ J. F. J. Todd and G. Lawson, *MTP International Review of Science, Physical Chemistry, Mass Spectrometry*, Series Two, Vol. 5, edited by A. Maccoll, Butterworths, London (1975).

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, 33, 101 (1980) and references cited within.

¹⁰ D. R. Denison, *J. Vac. Sci. Technol.*, 8, 266 (1971).

A. Finite Length of the Electrode Structure. The differential equations were derived under the assumption that the electrode structure is infinitely long. Real electrode structures are not infinitely long and so the electromagnetic fields are not functions of x and y alone but also depend on z ; i.e., they do not begin and end abruptly at the extremities of the electrode structure but extend at either end of the electrode structure giving rise to what is termed fringing fields. Fringing fields have been neglected in these derivations but for an actual mass filter these fields may be important.⁷ The assumption of infinite length was implicitly made when the potential was assumed to be independent of the z -coordinate.

B. Image Force on Ions. If an ion with a charge e is placed near an infinite conducting sheet at ground potential, the field of the ion will cause the free charges within the conductor to move in such a way that the field within the conductor is zero. These induced charges on the conductor will attract the ion to the conductor with a force,¹³

$$F = \frac{1}{4\pi\epsilon_0} \frac{e^2}{(2d)^2},$$

where d is the distance from the charge to the conducting sheet. It is as if there were an image charge of opposite polarity on the other side of the conductor, thus the name "image force" is used. Similarly, a charge in a conducting hollow sphere (not at the center) will be attracted to the nearest point of the conductor.¹³ For the geometry of the infinite sheet or sphere, the force on the ion is non-zero and this suggests that the force for an ion moving in the multipole geometries considered here is non-zero. The forces due to the induced charges on the conductor have been neglected in going from Equations M2 to M3; the radiofrequency source allows charge to flow to and from the electrode structure and so Equation M3 is not valid in the region of space which includes the electrode structure. In typical computer trajectory calculations, the ion is assumed to be lost once it hits the electrode.²³ Because of this so called "image force," the ions are more properly lost when they get to within a certain distance of the electrode structure.

C. E Fields Induced by Ions. Electric forces between ions may occur within the vacuum region enclosed by the pole pieces when an ion creates an electric field E at the site of a second ion. The second ion is thus acted upon by an electric force according to Coulomb's law.

⁷ P. H. Dawson (Editor), *Quadrupole Mass Spectrometry and Its Applications*, Elsevier, Amsterdam (1976).

¹³ E. M. Pugh and E. W. Pugh, *Principles of Electricity and Magnetism*, Addison-Wesley Publishing Co., Reading, MA (1960).

²³ J. E. Campana and P. C. Jurs, *Int. J. Mass Spectrom. Ion Phys.*, **33**, 119 (1980).

D. B Fields Induced by Ions. The movement of one ion generates a **B** field associated with the movement of that ion and if a second ion moves in the **B** field generated by the first ion, it will feel a force due to the **B** field of the first ion providing \mathbf{v} is not parallel to **B**. This force is neglected in the derivation given here. The forces in B, C, and D were neglected when \mathbf{J} and ρ were set equal to zero in Section I in going from Equation M2 to M3. These latter two forces discussed in C and D can be collectively termed space charge effects.

E. Presence of B Fields on Computing the E Field. The **E** field computed from the potential is only approximately correct because the term with $\frac{\partial \mathbf{B}}{\partial t}$ has been neglected in the second equation of Equation M5. At high enough frequencies, or with a mass filter with very large dimensions, the **E** field computed from the potential will be significantly in error and this would result in significant error in the differential equation describing the ion motion.

F. Presence of B Field on Computing the Force of the Ion. The fourth equation of Equations M3 shows that a changing **E** field generates a **B** field and from the Lorentz force law this **B** field exerts a force on the ion. Unless the ion is moving close to the speed of light, this force is usually negligible compared to the **E** field. It is reasonable to neglect this term for practical applications.

G. Radiation by the Accelerated Ion. A consequence of Maxwell's equations is that an accelerating charge gives off electromagnetic radiation.¹⁷ An accelerating charge requires an effective force to help balance the energy radiated. This force, which is proportional to the acceleration of the ion,¹⁷ has been neglected in these derivations.

The approximations discussed in E, F, and G were introduced as a consequence of dropping the time dependence of the **E** and **B** fields in going from Equations M3 to M4.

H. Ion Neutral Interaction. In the normal operation of a mass filter, ions may interact with residual gas in the chamber. It has been suggested²⁴ that this force can be represented as a viscous drag on the motion of the ion. The viscous force, proportional to the speed of the ion has been neglected in the derivation of the equations given here. At the normal operating pressures of mass filters (10^{-5} mm Hg), the mean free path of a particle is greater than 4.0×10^{-3} m.

¹⁷ J. D. Jackson, *Classical Electrodynamics*, John Wiley and Sons, Inc., New York (1962).

²⁴ N. R. Whetten, *J. Vac. Sci. Technol.*, 11, 515 (1974).

I. Gravitational Interaction. The gravitational interaction has been neglected. Because of the small amount of time an ion spends traversing a quadrupole mass filter, this effect is small for such a device and is expected to be more important in ion storage devices (three-dimensional mass filter).⁷

J. Relativistic Effects. Non-relativistic laws of mechanics are used in the method described in Section II. Since the fastest ions in a quadrupole mass filter move slowly⁹ ($v/c < 10^{-4}$) compared to the speed of light, the errors introduced by using non-relativistic mechanics are expected to be small.

V. APPLICATION TO SOME MULTIPOLE GEOMETRIES

The method described in Section III will be demonstrated here to obtain the potential functions and the differential equations of ion motion for the dipole, quadrupole, hexapole, octapole, and decapole electrode geometries.

A. The Dipole Field. The variable z is raised to the first power to obtain:

$$U_1(x,y) = x$$

$$V_1(x,y) = y.$$

Since $\nabla^2 U_1(x,y) = 0$, the function $U_1(x,y)$ forms the basis for a potential function in charge-free space. Its equipotential surfaces are illustrated in Figure 2. This leads to a model in which there are two plane sheets: one at $x = r$ and one at $x = -r$ with applied potentials of $\phi_0/2$ and $-\phi_0/2$, respectively. The potential function $\phi(x,y) = K_1 U_1(x,y)$ can be deduced to be

$$\phi(x,y) = \frac{\phi_0}{2} \frac{x}{r_0} \quad ; \quad -r_0 \leq x \leq r_0$$

if it is to satisfy both Laplace's equation and the boundary conditions $[\phi(\pm r_0, y) = \pm \phi_0/2]$ in Equation 20. With ϕ_0 given by Eq. 22, Newton's law Eq. 21 becomes:

$$\begin{aligned} m \frac{d^2 x}{dt^2} + \frac{e}{2r_0} (\phi_{DC} - \phi_{AC} \cos \omega t) &= 0 \\ m \frac{d^2 y}{dt^2} &= 0. \end{aligned} \quad (28)$$

⁷ P. H. Dawson (Editor), *Quadrupole Mass Spectrometry and Its Application*, Elsevier, Amsterdam (1976).

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, 33, 101 (1980) and references cited within.

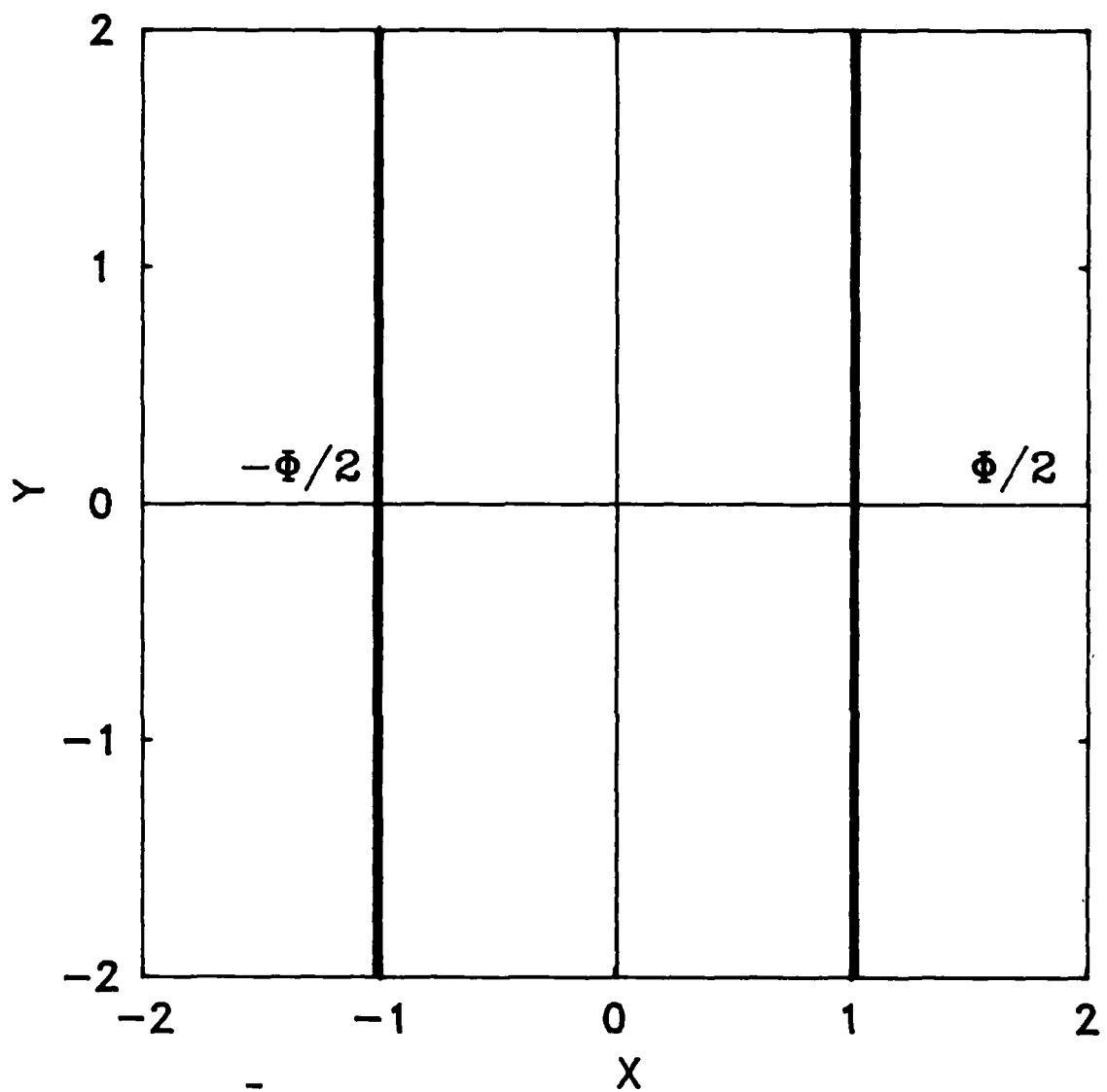


Figure 2. Dipole geometry.

The positive and negative equipotential surfaces consists of two plane sheets separated by a distance $2r_0$. The surfaces at $x=r_0$ and $x=-r_0$ are at potentials $\phi_0/2$ and $-\phi_0/2$.

B. The Quadrupole Field. The function z^n for $n=2$ is evaluated to obtain:

$$U_2(x,y) = x^2 - y^2$$

$$V_2(x,y) = 2xy.$$

Since $\nabla^2 U_2(x,y) = 0$, the function $U_2(x,y)$ is the basis for a possible potential function in charge-free space. Its equipotential surfaces are illustrated in Figure 3. Each of the four hyperbolic pole pieces have the same geometry and hence the structure is unchanged under 90° rotation. The pole pieces lying on the x-axis are arbitrarily chosen to have positive applied potentials $+\phi_o/2$ and the pole pieces lying on the y-axis are arbitrarily chosen to have negative applied potentials $-\phi_o/2$. The potential function $\phi(x,y)$ can be deduced to be

$$\phi(x,y) = \frac{\phi_o}{2r_o^2} (x^2 - y^2).$$

It is readily verified that this potential function satisfies both Laplace's equation and the boundary conditions, Equation 20 [eg. $\phi(r_o,0) = \phi_o/2$ and $\phi(0,r_o) = -\phi_o/2$]. With ϕ_o given by Equation 22, Newton's law becomes:

$$\begin{aligned} m \frac{d^2 x}{dt^2} + \frac{e}{r_o^2} (\phi_{DC} - \phi_{AC} \cos \omega t) x &= 0 \\ m \frac{d^2 y}{dt^2} - \frac{e}{r_o^2} (\phi_{DC} - \phi_{AC} \cos \omega t) y &= 0. \end{aligned} \quad (29)$$

The electric potential and the differential equation obtained here agree exactly with those derived elsewhere by various other methods.⁹ Equations 29 are of the well studied Mathieu-type equation.^{4,6}

⁴ F. M. Arscott, *Periodic Differential Equations*, The Macmillan Co., New York (1964).

⁵ N. W. McLachlan, *Theory and Application of Mathieu Functions*, Oxford University Press, New York (1947).

⁶ Computation Laboratory, *Tables Relating to Mathieu Functions*, U.S. Bureau of Standards, Columbia University Press, New York (1951).

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, **33**, 101 (1980) and references cited within.

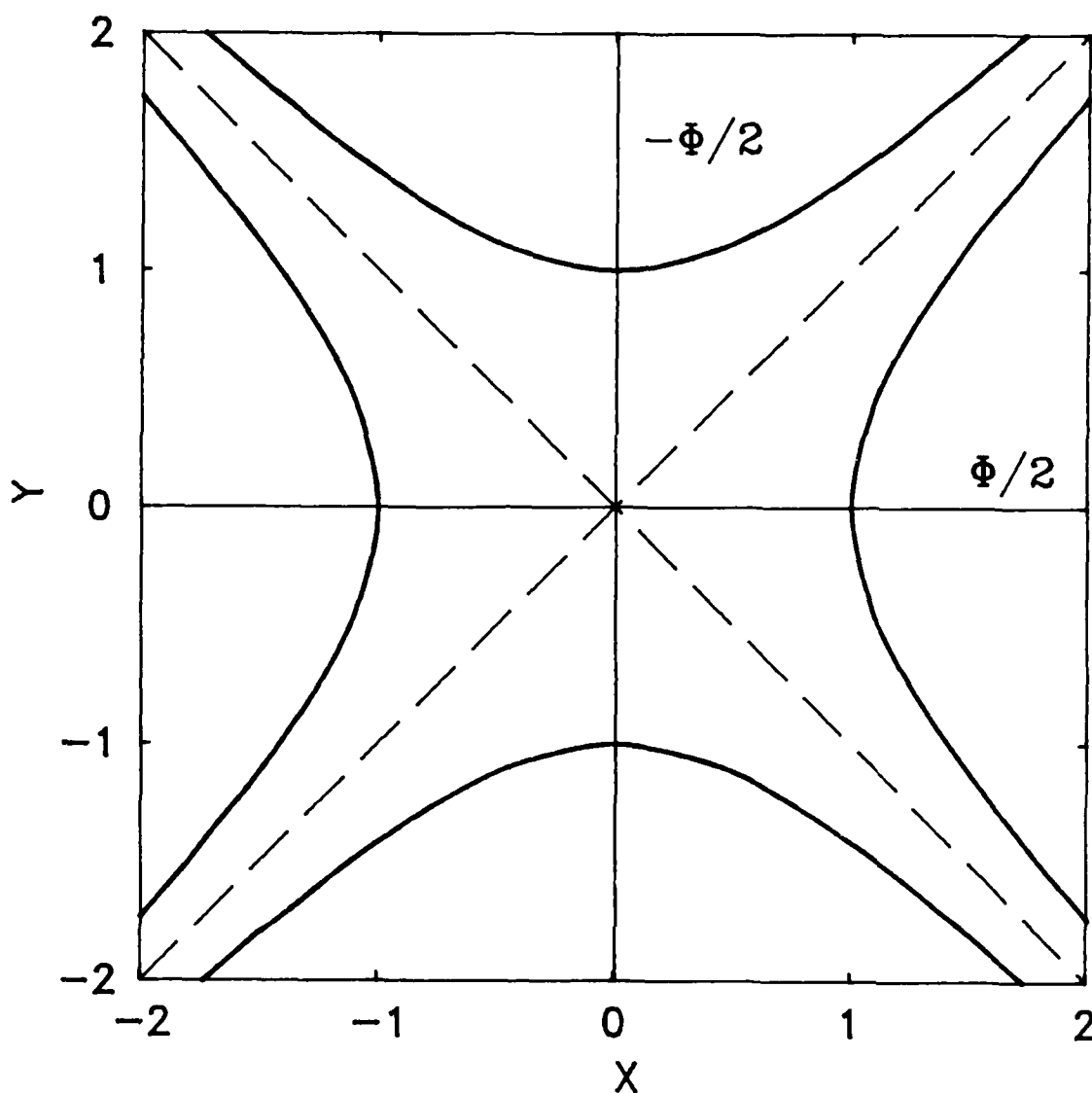


Figure 3. Quadrupole geometry.
 The positive and negative equipotentials consist of four surfaces with an inscribed radius of r_0 . The equations of the equipotential surfaces are $\phi(x,y) = (\phi_0/2r_0^2)(x^2 - y^2)$.

C. The Hexapole Field. The function z^n for $n=3$ is evaluated to obtain:

$$U_3(x,y) = x^3 - 3xy^2$$

$$V_3(x,y) = 3x^2y - y^3.$$

Since $\nabla^2 U_3(x,y) = 0$, the function $U_3(x,y)$ is the basis for a possible potential function in charge-free space. Its equipotential surfaces are illustrated in Figure 4. Each of the six pole pieces have the same shape and so the structure is unchanged under a 60° rotation. Similarly, as in the previous examples, the potential function $\phi(x,y)$ can be deduced to be

$$\phi(x,y) = \frac{\phi_o}{2r_o^3} (x^3 - 3xy^2).$$

It is readily verified that this function satisfies both Laplace's equation and the boundary conditions. With ϕ_o given by Equation 22, Newton's law becomes:

$$\begin{aligned} m \frac{d^2 x}{dt^2} + \frac{3}{2} \frac{e}{r_o^3} (\phi_{DC} - \phi_{AC} \cos \omega t) (x^2 - y^2) &= 0 \\ m \frac{d^2 y}{dt^2} - \frac{3e}{r_o^3} (\phi_{DC} - \phi_{AC} \cos \omega t) xy &= 0. \end{aligned} \quad (30)$$

D. The Octapole Field. The function z^n for $n=4$ is evaluated to obtain:

$$U_4(x,y) = x^4 - 6x^2y^2 + y^4$$

$$V_4(x,y) = 4xy(x^2 - y^2).$$

Since $\nabla^2 U_4(x,y) = 0$, the function $U_4(x,y)$ is the basis for a possible potential function in charge-free space. Its equipotential surfaces are illustrated in Figure 5. Each of the eight pole pieces have the same shape and so the structure is unchanged under a 45° rotation. Similarly, as in the previous examples, the potential $\phi(x,y)$ can be deduced to be

$$\phi(x,y) = \frac{\phi_o}{2r_o^4} (x^4 - 6x^2y^2 + y^4).$$

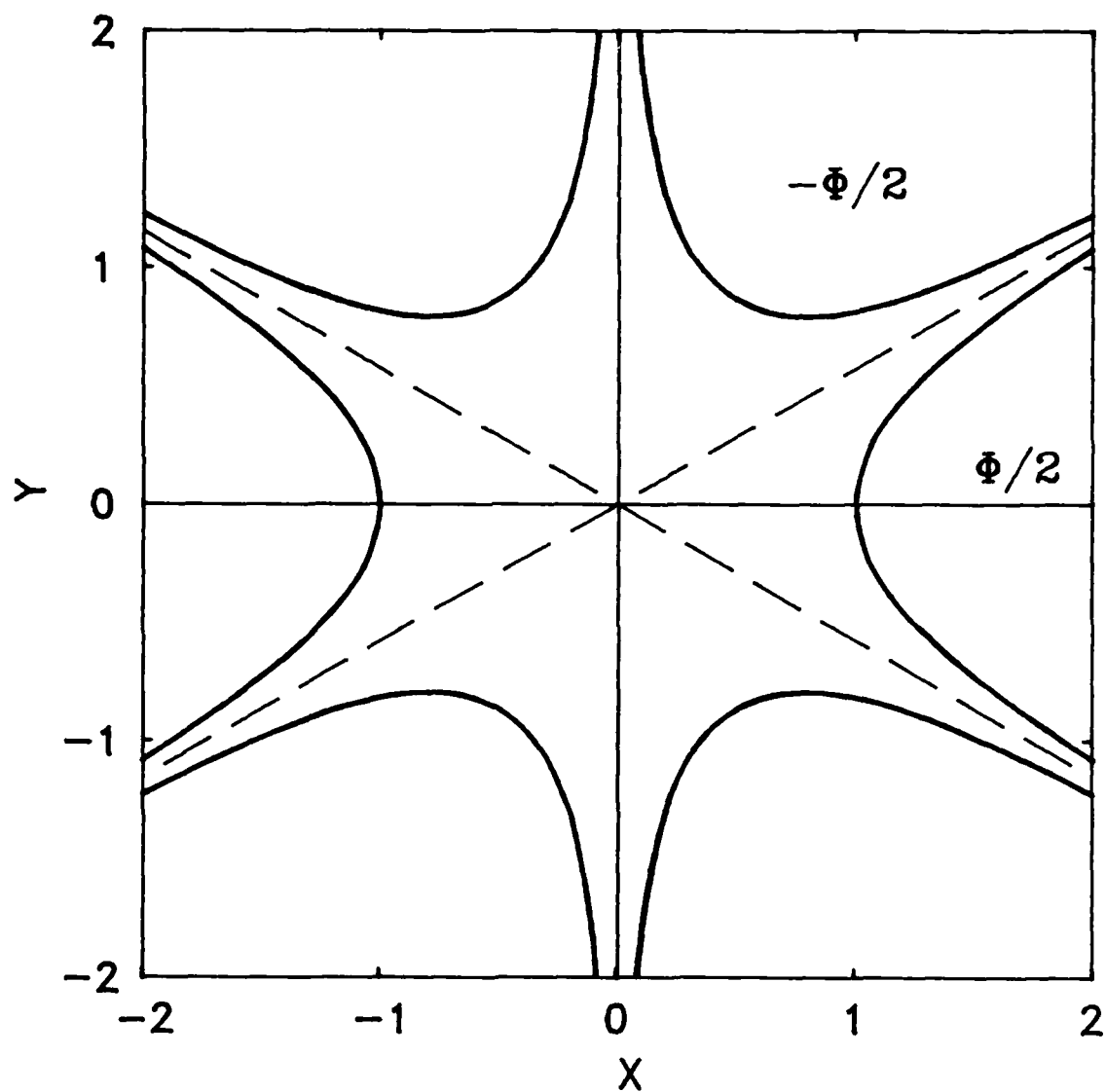


Figure 4. Hexapole geometry.
The positive and negative equipotentials consist of six surfaces with an inscribed radius of r_0 . The equation of the equipotential surfaces are $\phi(x,y) = (\phi_0/2r_0^3) (x^3 - 3xy^2)$.

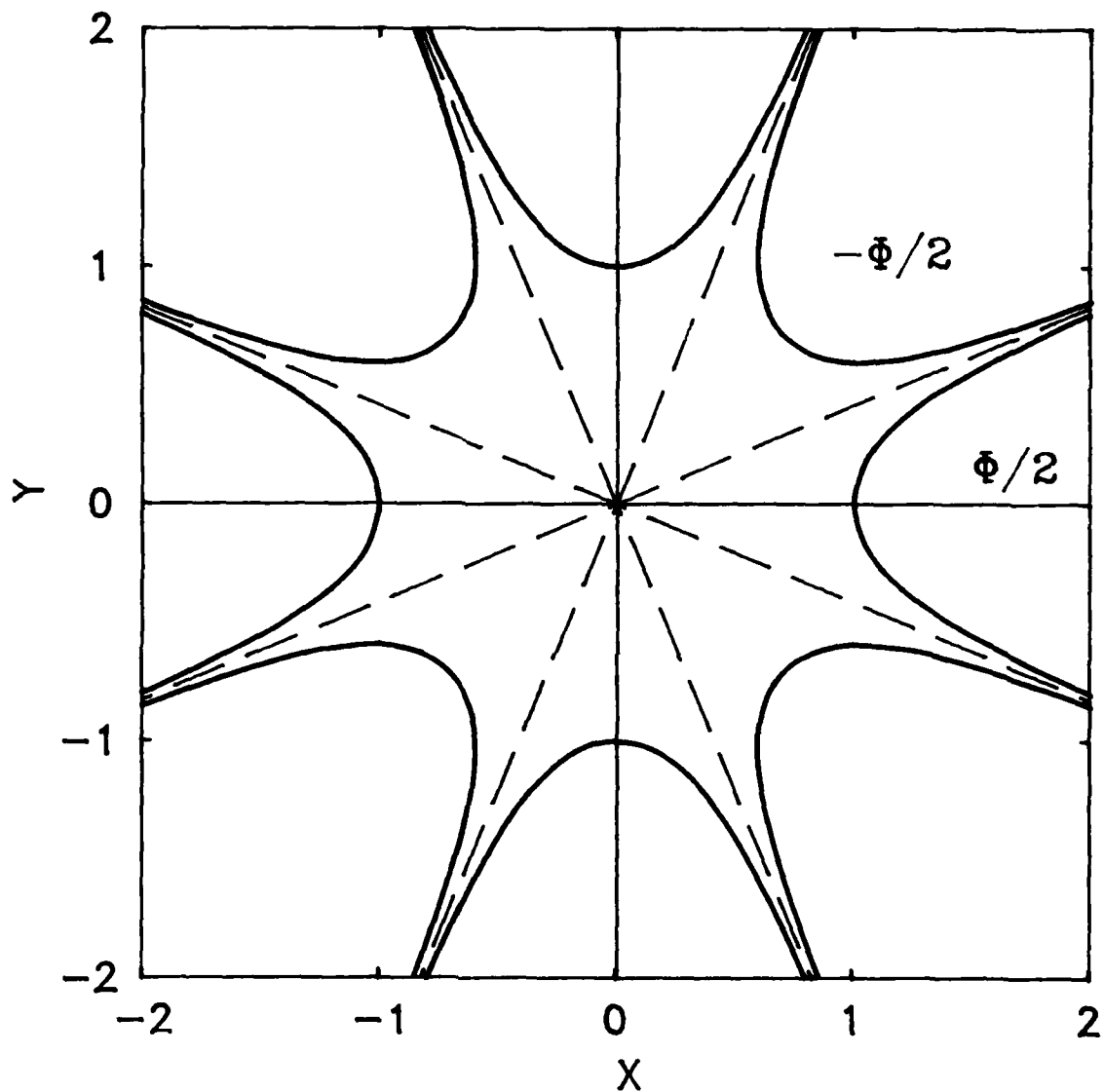


Figure 5. Octapole geometry.

The positive and negative equipotentials consists of eight surfaces with an inscribed radius of r_0 . The equation of the equipotential surfaces are $\phi(x,y) = (\phi_0/2r_0^4) (x^4 - 6x^2y^2 + y^4)$.

It is readily verified that this function satisfies Laplace's equation and the boundary conditions. With ϕ_0 by Equation 22, Newton's law becomes:

$$\begin{aligned} m \frac{d^2 x}{dt^2} + \frac{2e}{r_0^4} (\phi_{DC} - \phi_{AC} \cos \omega t) (x^3 - 3xy^2) &= 0 \\ m \frac{d^2 y}{dt^2} - \frac{2e}{r_0^4} (\phi_{DC} - \phi_{AC} \cos \omega t) (3x^2y - y^3) &= 0. \end{aligned} \quad (31)$$

E. The Decapole Field. The function z^n for $n=5$ is evaluated to obtain:

$$U_5(x,y) = x^5 - 10x^3y^2 + 5xy^4$$

$$V_5(x,y) = y^5 - 10x^2y^3 + 5x^4y.$$

Since $\nabla^2 U_5(x,y) = 0$, the function $U_5(x,y)$ is the basis for a possible potential function in charge-free space. Its equipotential surfaces are illustrated in Figure 6. Each of the 10 pole pieces have the same shape, and so the structure is unchanged under a 36° rotation. Similarly, as in the previous examples, the potential function $\phi(x,y)$ can be deduced to be

$$\phi(x,y) = \frac{\phi_0}{2r_0^5} (x^5 - 10x^3y^2 + 5xy^4).$$

It is readily verified that this function satisfies Laplace's equation and the boundary conditions. With ϕ_0 given by Equation 22, Newton's law becomes:

$$\begin{aligned} m \frac{d^2 x}{dt^2} + \frac{5e}{2r_0^5} (\phi_{DC} - \phi_{AC} \cos \omega t) (x^4 - 6x^2y^2 + y^4) &= 0 \\ m \frac{d^2 y}{dt^2} - \frac{10e}{r_0^5} (\phi_{DC} - \phi_{AC} \cos \omega t) (x^3y - xy^3) &= 0. \end{aligned} \quad (32)$$

F. Fields of Geometry Higher Than the Decapole. The method illustrated in these examples can be used without difficulty for finding the differential equation of an ion for $n > 5$, where n is an integer.

G. Generalization of Differential Equations to an Arbitrary Phase. The alternating component at time $t=0$ is ϕ_{AC} in the differential Equations 28-32. Ions may enter the electric field at any time where the alternating component can have any value between $+\phi_{AC}$ and $-\phi_{AC}$. Thus Equations 28-32 may be written more generally by replacing ωt with $\omega t + \delta$ where $0 \leq \delta < 2\pi$.

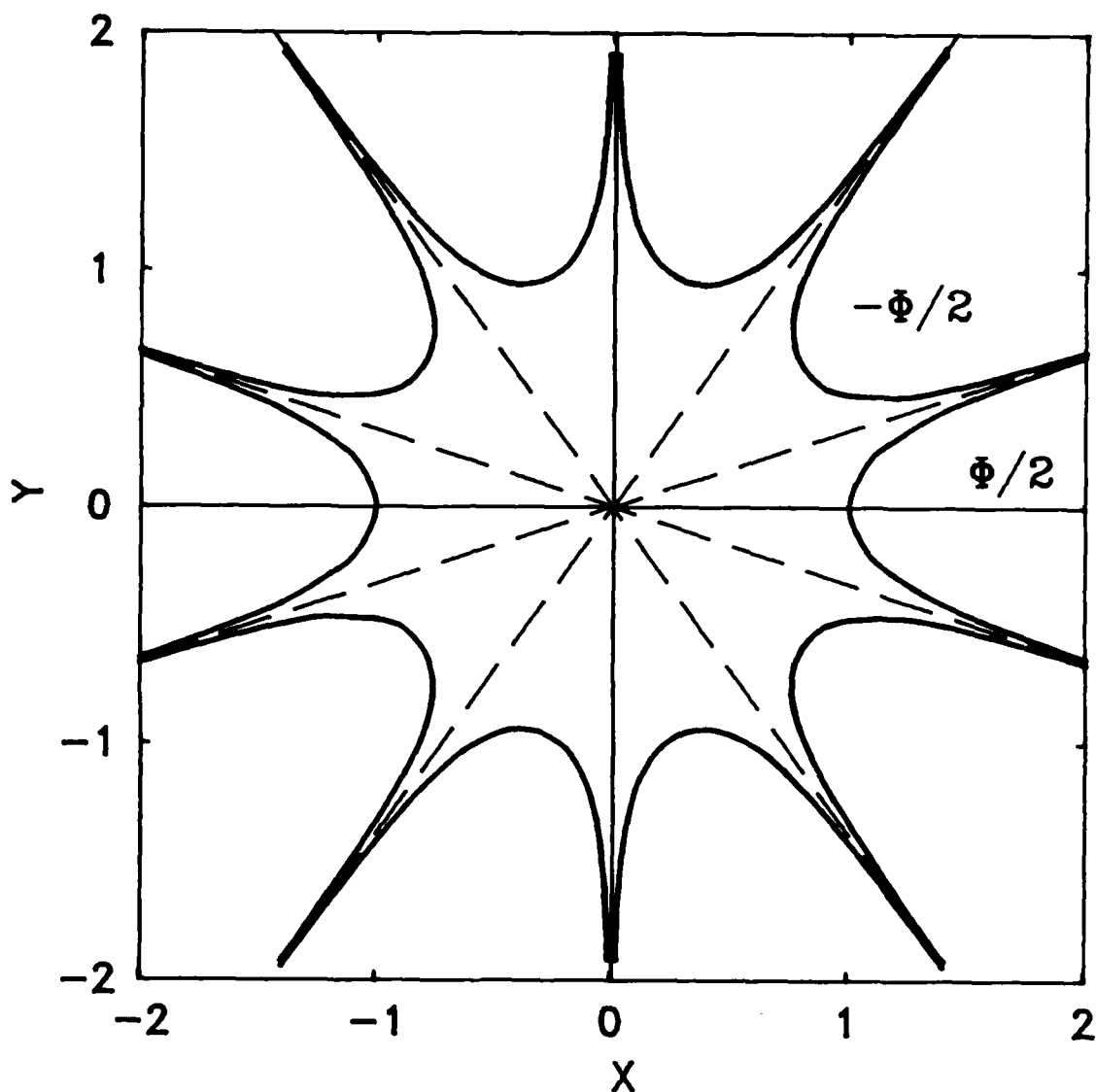


Figure 6. Decapole geometry.

The positive and negative equipotentials consist of 10 surfaces with an inscribed radius of r_0 . The equations of the equipotential surfaces are $\phi(x,y) = (\phi_0/2r_0^5)(x^5 - 10x^3y^2 + 5xy^4)$.

H. Redundancy of the V Function. The function $V_n(x,y)$ defined in Equation 25 also satisfies Laplace's equation; i.e., $\nabla^2 V_n(x,y) = 0$. This can be seen readily by taking the sum of the partial derivative of Equation 26a with respect to y and the partial derivative of Equation 26b with respect to x . Since $V_n(x,y)$ satisfies Laplace's equation, it might seem that the equipotentials $V_n(x,y) = \phi_0/2$ and $V_n(x,y) = -\phi_0/2$ would generate different surfaces than the corresponding equations for the function $U_n(x,y)$.

The surfaces defined by $V_n(x,y) = \pm \phi_0/2$ are the same as those defined by $U_n(x,y) = \pm \phi_0/2$ respectively except rotated by an angle α_n . This is seen by expressing $(x + iy)^n$ in polar coordinates

$$(x + iy)^n = (re^{i\theta})^n = r^n(\cos n\theta + i \sin n\theta).$$

Comparison of this last equation with Equation 25 shows

$$U_n(x,y) = r^n \cos n\theta \quad (33a)$$

$$V_n(x,y) = r^n \sin n\theta. \quad (33b)$$

Define a primed coordinate system rotated by an amount $\alpha_n = \pi/2n$ relative to the unprimed $\theta' = \theta - \frac{\pi}{2n}$

In the primed coordinate system

$$V_n = r^n \sin n\left(\theta' + \frac{\pi}{2n}\right) = r^n \cos n\theta'. \quad (34)$$

Since the form of Equation 34 is the same as Equation 33a, the use of the function $V_n(x,y)$ generates the same apparatus as the function $U_n(x,y)$ rotated by an angle $\alpha_n = \frac{\pi}{2n}$.

VI. MULTIPOLE GEOMETRIES AS MASS FILTERS

The methods presented in the preceding sections yield the differential equations of motion for ions in time-varying electric fields. A system functions as a mass filter if it passes ions in a certain mass interval, rejects all other ions, and the mass interval is under the control of the experimenter.

A. The Dipole Field. The equation of motion for the x and y directions can be integrated directly:

$$x = A+Bt - \frac{e\phi_{DC}}{4mr_0} t^2 - \frac{e\phi_{AC} \cos \omega t}{2mr_0 \omega^2}$$

$$y = v_{y_0} t + y_0 \quad (35)$$

Here A and B are constants which depend on the initial x-coordinate and x-velocity, respectively, and y_0 and v_{y_0} are the initial y-coordinate and y-velocity. It is apparent from Equations 35 that the motion is unstable in both the x- and y-coordinate directions for all initial conditions. Thus, the dipole field with sinusoidal voltage is unsuitable as a mass filter.

B. The Quadrupole Field. It is well known that once can choose ϕ_{DC} and ϕ_{AC} such that there is stability for both the x- and y-directions for a narrow range of mass values. The quadrupole geometry is suitable as a mass filter.^{7,9}

C. The Hexapole, Octapole, and Decapole Fields. The differential equations for these three geometries are not readily integrated. It has been shown that numerical methods can be used successfully to integrate equations of motion, when motion in one coordinate direction is not independent of the motion in the other direction.¹⁰ The utility of such systems as mass filters awaits the numerical integration of the equation of motion and is the subject of future research.

VII. SUMMARY

A general method for finding the differential equations of ion motion in electromagnetic fields has been presented and applied to five different multipole geometries. The fundamental physics and the approximations used in obtaining the differential equations have been reviewed so that limitations in the analytical theory can be appreciated better.

⁷ P. H. Dawson (Editor), *Quadrupole Mass Spectrometry and Its Applications*, Elsevier, Amsterdam (1976).

⁸ J. F. J. Todd and G. Lawson, *MTP International Review of Science, Physical Chemistry, Mass Spectrometry*, Series Two, Vol. 5, edited by A. Maccoll, Butterworths, London (1975).

⁹ J. E. Campana, *Int. J. Mass Spectrom. Ion Phys.*, **33**, 101 (1980) and references cited within.

¹⁰ D. R. Denison, *J. Vac. Sci. Technol.*, **8**, 266 (1971).

Today the quadrupole mass analyzer is the most widely used mass analyzer for low resolution applications. Typically, mass filters are used in laboratory environments where simplicity, compactness, economy, absence of magnetic fields, and/or the capability of fast scan rates (especially for chromatographic combinations) are important. Thus, an improvement in resolution/transmission qualities of electric RF mass filters would enable this widely used mass spectrometer to take a larger role in analytical laboratories and in basic research.

Other design considerations besides resolution/transmission characteristics are important. If mass filters could be made which are smaller, more rugged, and less susceptible to vibration with reduced power requirements while being maintained more easily, they might find application outside the laboratory. Possible applications include surveying for natural resources, pin-pointing sources of industrial and natural pollutants and the detection of explosive materials.

ABBREVIATIONS AND SYMBOLS

A	Any vector field
B	Magnetic field vector
B₀	Maximum amplitude of the B field
c	Speed of light
D	Electric displacement vector
d	Distance from a point charge to a conducting sheet
E	Electric field vector
E₀	Maximum amplitude of E field
e	Electron charge
F	Force vector
H	Magnetic field intensity or magnetic field strength vector
\hat{i}	Unit vector along x-axis
J	Current density vector
\hat{j}	Unit vector along y-axis
K	A constant, related to the dimensions of the electrode structure and the applied electrode voltage
\hat{k}	Unit vector along z-axis
ℓ	Length of the electrode structure
M	Magnetization vector
m	Magnetic polarization vector

m	Mass
\mathbf{P}	Polarization vector
RF	Radiofrequency
\mathbf{r}	Radius vector
r_o	Inscribed radius of the electrode structure
t	Time
U_n	A real function satisfying Laplace's equation
$U(\mathbf{r})$	A potential energy function
V_n	An imaginary part of a function that satisfies Laplace's equation
\mathbf{v}	Velocity vector
α	Radian measure
δ	Radian measure
ϵ	The permittivity
ϵ_o	The permittivity of free space
θ	Radian measure
λ	Wavelength
μ	Permeability
μ_o	Permeability of free space
ν	Frequency
ρ	Charge density
$\phi(x,y,z)$	A potential function

ϕ	A scalar function of position or applied voltage
χ_e	Polarizability or the electric susceptibility
χ_m	Magnetic susceptibility
ω	Angular frequency
∇	"del operator"
∇^2	The Laplacian
∂	Backcurling delta (partial derivative sign)
\oint	Contour integral

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